Applications of Jarzynski's relation in lattice gauge theories

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Based on:

M. Caselle, G. Costagliola, A. N., M. Panero and A. Toniato
arXiv:1604.05544 [hep-lat]

Free-energy differences in LGTs

In lattice gauge theories the expectation values of a large set of physical quantities is *naturally* related to the computation (via Monte Carlo simulations) of free-energy differences.

For example:

- equilibrium thermodynamics (pressure)
- 't Hooft loops
- magnetic susceptibility

In many cases the calculation of ΔF is a **computationally challenging** problem: this motivates the search for new methods and algorithms.

In this talk a **novel** (in LGTs) method to calculate *directly* free-energy differences based on Jarzynski's relation is presented. In general we are interested in any case in which we compute the ratio of partition functions of **physical systems**, i.e. expressed in terms of **well-defined** fields and couplings.

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1. Jarzynski's relation
2. Benchmark study I: interface free energy in $\mathbb{Z}_2$ gauge model
3. Benchmark study II: pressure in $\mathrm{SU}(2)$ gauge theory
4. Future applications

Jarzynski's equality - I

Jarzynski's equality [Jarzynski, 1997] relates the exponential statistical average of the work done on a system during a non-equilibrium process with the difference between the initial and the final free energy of the system.
For an isothermal transformation it can be written as

$$\left\langle \exp\left(-\frac{W(\lambda_i, \lambda_f)}{T}\right)\right\rangle = \exp\left(-\frac{\Delta F}{T}\right)$$

The evolution of the system is performed by changing (continuously or discretely) a chosen set λ of one or more parameters, such as the couplings or the temperature of the system.
In each step of the process the value of λ is changed and the system is brought **out of equilibrium**.

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Jarzynski's equality - II

$$\left\langle \exp\left(-\frac{W(\lambda_i,\lambda_f)}{T}\right)\right\rangle = \exp\left(-\frac{\Delta F}{T}\right)$$

- on the r.h.s. $\exp\left(-\frac{\Delta F}{T}\right) = \frac{Z(T,\lambda_f)}{Z(T,\lambda_i)}$ where $\Delta F = F(\lambda_f) - F(\lambda_i)$
- $W(\lambda_i,\lambda_f)$ is the **work** made on the system to change the control parameter from λ_i to λ_f. If the transformation is discrete (like a Markov chain in MC simulations), then the process is divided into N steps and the total work is

$$W(\lambda_i \equiv \lambda_0, \lambda_f \equiv \lambda_N) = \sum_{n=0}^{N-1} \left(H_{\lambda_{n+1}}[\phi_n] - H_{\lambda_n}[\phi_n]\right)$$

  where ϕ_n is the configuration of the variables of the system at the n-th step of the transformation
- the $\langle ... \rangle$ indicates the **average** on all possible realizations of the non-equilibrium transformation

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Jarzynski's equality - Comments

- The equality requires no particular assumptions and holds under very general conditions (e.g. the detailed balance condition for Markov chains)
- It can be extended for non-isothermal transformations [Chatelain, 2007]
- In Monte Carlo simulations we can control
  - N, the number of steps for each transformation between initial and final value of the parameter λ
  - n_r, the number of "trials", i.e. realizations of the non-equilibrium transformation
- A systematic **discrepancy** appears between the results of the 'direct' ($\lambda_i \to \lambda_f$) and the 'reverse' ($\lambda_f \to \lambda_i$) transformation. One has to choose a suitable combination of N and n_r in order to obtain convergence.

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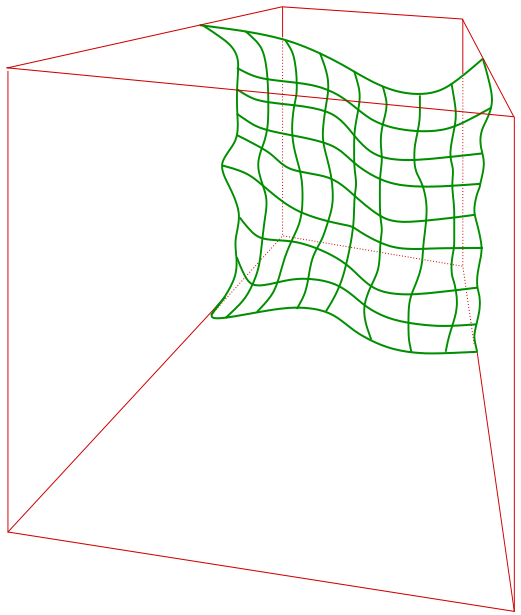
Benchmark study I: interface free energy in $\mathbb{Z}_2$ gauge model

Interfaces in the $\mathbb{Z}_2$ gauge model

Why study interfaces?

- experimental applications in condensed matter systems
- appear in many contexts also in HEP ("domain walls" at finite T, 't Hooft loops)
- also related to flux tubes in confining gauge theories which can be studied with string-theory tools



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The $\mathbb{Z}_2$ gauge model in 3 dimensions is the simplest lattice gauge theory in which to study interfaces: it is described by a Wilson action with $\mathbb{Z}_2$ variables and possesses a **confining** phase for small values of the inverse coupling β_g.

It can be exactly rewritten through the Kramers-Wannier duality as the 3-dimensional Ising model on the **dual** lattice:

$$H = -\beta \sum_{x,\mu} J_{x,\mu}\, \sigma_x\, \sigma_{x+a\hat{\mu}}$$

where

$$\beta = -\frac{1}{2} \ln \tanh \beta_g$$

Interface free energy

To create an interface we induce a **frustration** on the system, by imposing $J_{x,\mu} = -1$ only for the couplings in a specific slice of the lattice (and only in one direction) and setting the remaining ones to 1.

The **free energy** associated with this interface can be expressed as the ratio between two partition functions:

- one where all couplings are set to $J_{x,\mu} = 1$ (**periodic** boundary conditions)
- another in which the couplings between the first and last slice in a specific direction μ are set to $J_{x,\mu} = -1$ (**antiperiodic** boundary conditions)

$$\frac{Z_a}{Z_p} = N_0 \exp(-F^{(1)})$$

where N_0 is the size of the lattice in the μ direction (an improved definition [Caselle et al., 2007] can be used to account for multiple interfaces in finite-size systems).

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Results in the $\mathbb{Z}_2$ gauge model

In order to compute the Z_a/Z_p ratio we can apply the Jarzynski's relation by gradually varying the $J_{x,\mu}$ parameter of the chosen slice from 1 to -1 (and viceversa):

$$J_{x,\mu}(n) = 1 - \frac{2n}{N}$$

where N is the total number of steps between periodic ($J_{x,\mu}(0) = 1$) and antiperiodic ($J_{x,\mu}(N) = -1$) boundary conditions.

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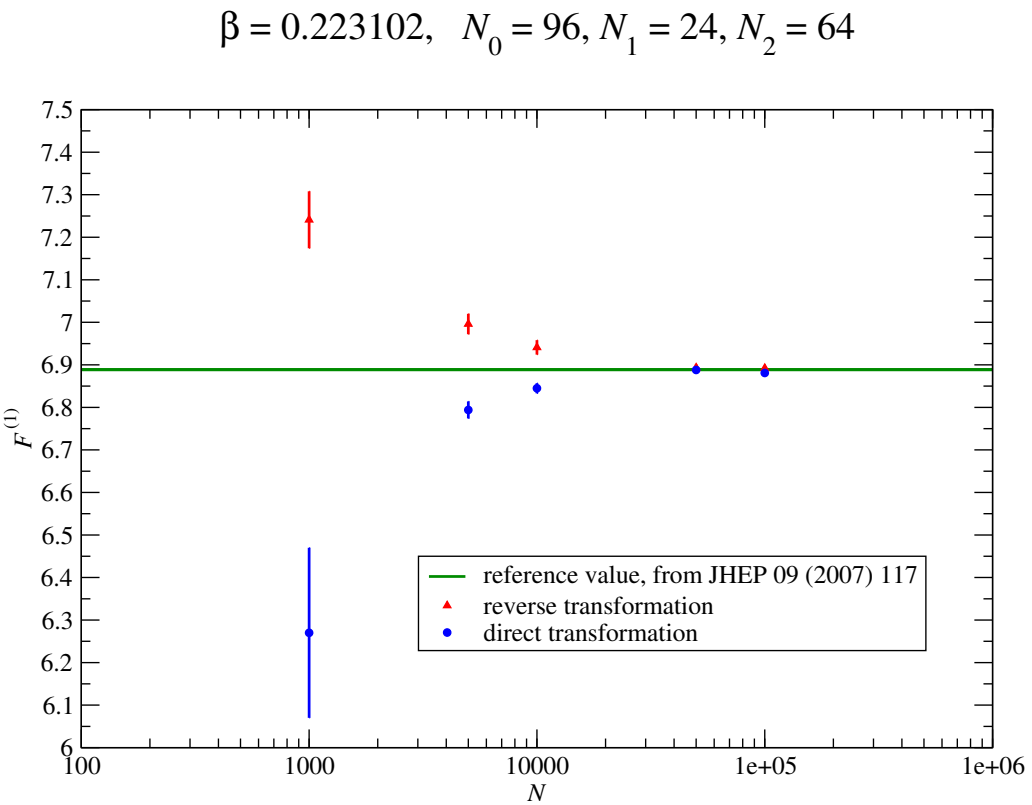

The results from 'direct' and 'reverse' transformations converge to older results when N is large enough.

The results obtained changing the interface size L can be compared with the analytical prediction of the effective string model.

Benchmark study II: pressure in $\mathrm{SU}(2)$ gauge theory

Equilibrium thermodynamics in non-Abelian gauge theories

- The thermal properties of QCD and QCD-like theories are particularly well suited for being studied on the lattice, due to non-perturbative nature of the deconfinement transition.

- The low-temperature phase ($T < T_c$) can be studied with great accuracy and lattice results close to the critical temperature can be compared with a gas of massive, non-interacting hadrons.

- For pure Yang-Mills theories this is even more dramatic and lattice data in the confining region have been compared in detail with the prediction of a glueball gas with an Hagedorn spectrum [Meyer, 2009; Borsányi et al., 2012; Caselle et al., 2015].

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Pressure on the lattice

On an hypercubic lattice of size $N_t \times N_s^3$, the temperature is determined by the inverse of the temporal extent (with periodic boundary conditions): $T = 1/(a(\beta_g)N_t)$. In practice, the temperature is controlled by the inverse coupling $\beta_g = \frac{2N_c}{g^2}$.

The **pressure** p in the thermodynamic limit equals the opposite of the free energy density

$$p \simeq -f = \frac{T}{V} \log Z(T, V)$$

and a common way to estimate it on the lattice is using the so-called "integral method" [Engels et al. (1990)]:

$$p(T) = \frac{1}{a^4} \frac{1}{N_t N_s^3} \int_0^{\beta_g(T)} d\beta_g' \frac{\partial \log Z}{\partial \beta_g'}$$

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Pressure with Jarzynski's relation

Jarzynski's relation gives us a direct method to compute the pressure: we can change the parameter β_g controlling the temperature T in a non-equilibrium transformation!

The **difference of pressure** between two temperatures T and T_0 is

$$\frac{p(T)}{T^4} - \frac{p(T_0)}{T_0^4} = \left(\frac{N_t}{N_s}\right)^3 \ln\langle e^{-W_{\mathrm{SU}(N_c)}}\rangle$$

with $W_{SU(N_c)}$ being the "work" made on the system:

$$W_{\mathrm{SU}(N_c)} = \sum_{n=0}^{N-1} \left[S_W(\beta_g^{(n+1)}, \hat{U}) - S_W(\beta_g^{(n)}, \hat{U}) \right];$$

here S_W is the standard Wilson action and $\hat{U}$ is a configuration of $\mathrm{SU}(N_c)$ variables on the links of the lattice.

Several values of this difference have been computed with this algorithm in the proximity of the deconfining transition (for temperatures $T < T_c$), using either $N = 1000$ or $N = 2000$ steps and $n_r = 30$ transformations for each point.

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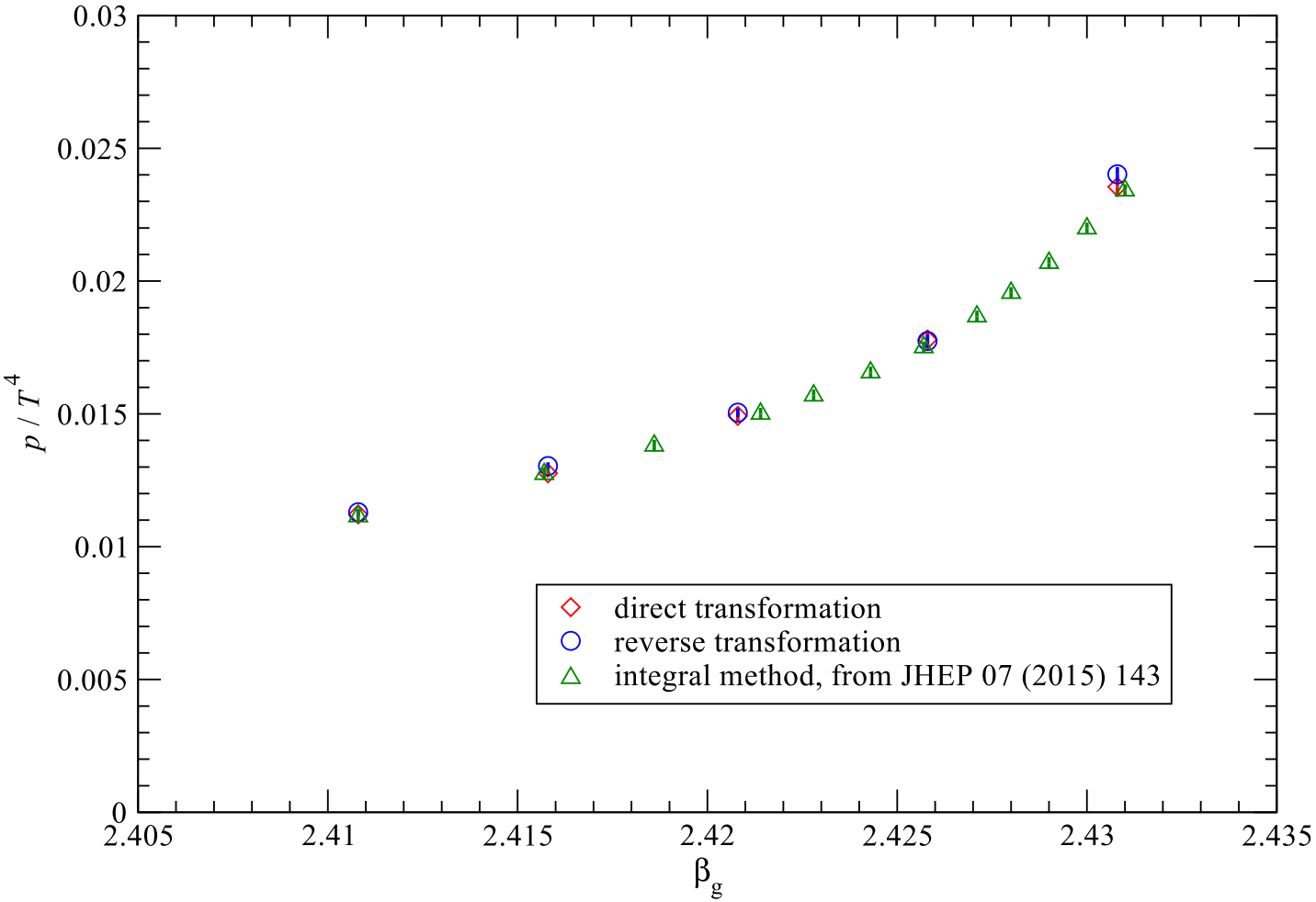
Preliminary results for the SU(2) model

Finite T simulations performed on $72^3 \times 6$ lattices. Temperature range is $\sim [0.9\,T_c, T_c]$.



Excellent agreement with integral method data [Caselle et al., 2015] but using a fraction of CPU time.

Some potential applications

- In principle there are no obstructions to the derivation of numerical methods based on Jarzynski's relation for fermionic algorithms, opening the possibility for many potential applications in full QCD

- One example is the calculation of the free energy density in QCD with a **background magnetic field** B, in order to measure the magnetic susceptibility of the strongly-interacting matter.

  Methods based on Jarzynski's relation can be applied in order to perform non-equilibrium transformations in which the field B itself is changed gradually.

- Another interesting application that we envision is in studies involving the **Schrödinger functional**: Jarzynski's relation could be used to compute changes in the transition amplitude induced by a change in the parameters that specify the initial and final states on the boundaries.

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Conclusions

Jarzynski's equality allows for new ways of computing free-energy differences in lattice gauge theories. A method based on this relation has been tested for the computation of two different physical quantities:

- the free energy of an interface in the $\mathbb{Z}_2$ gauge model
- the pressure in the confining region of the $\mathrm{SU}(2)$ gauge model

In both cases the method proved to be perfectly reliable with a suitable choice of N and n_r; moreover the computational efficiency is comparable and in many cases superior to standard methods.

Thank you for the attention!

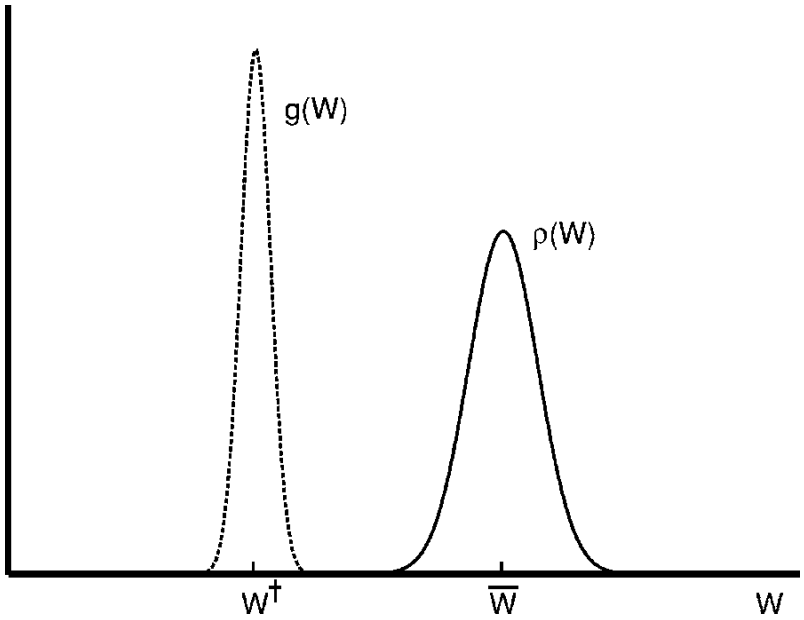
Effective string prediction

With this method (using $N \simeq 10^6$ steps and $n_r \simeq 10^3$ trials) we obtained high-precision results at fixed β and for different interface size L.

These results can be compared with the analytical prediction of the effective string model which describes the transverse fluctuations of the interface at low energy.

In particular, choosing the Nambu-Goto action as S_{eff}, one can look at the difference between numerical results and the NG prediction and examine its dependence on the size L of the interface, in order to understand the nature of the terms that do not arise from the NG low-energy expansion.

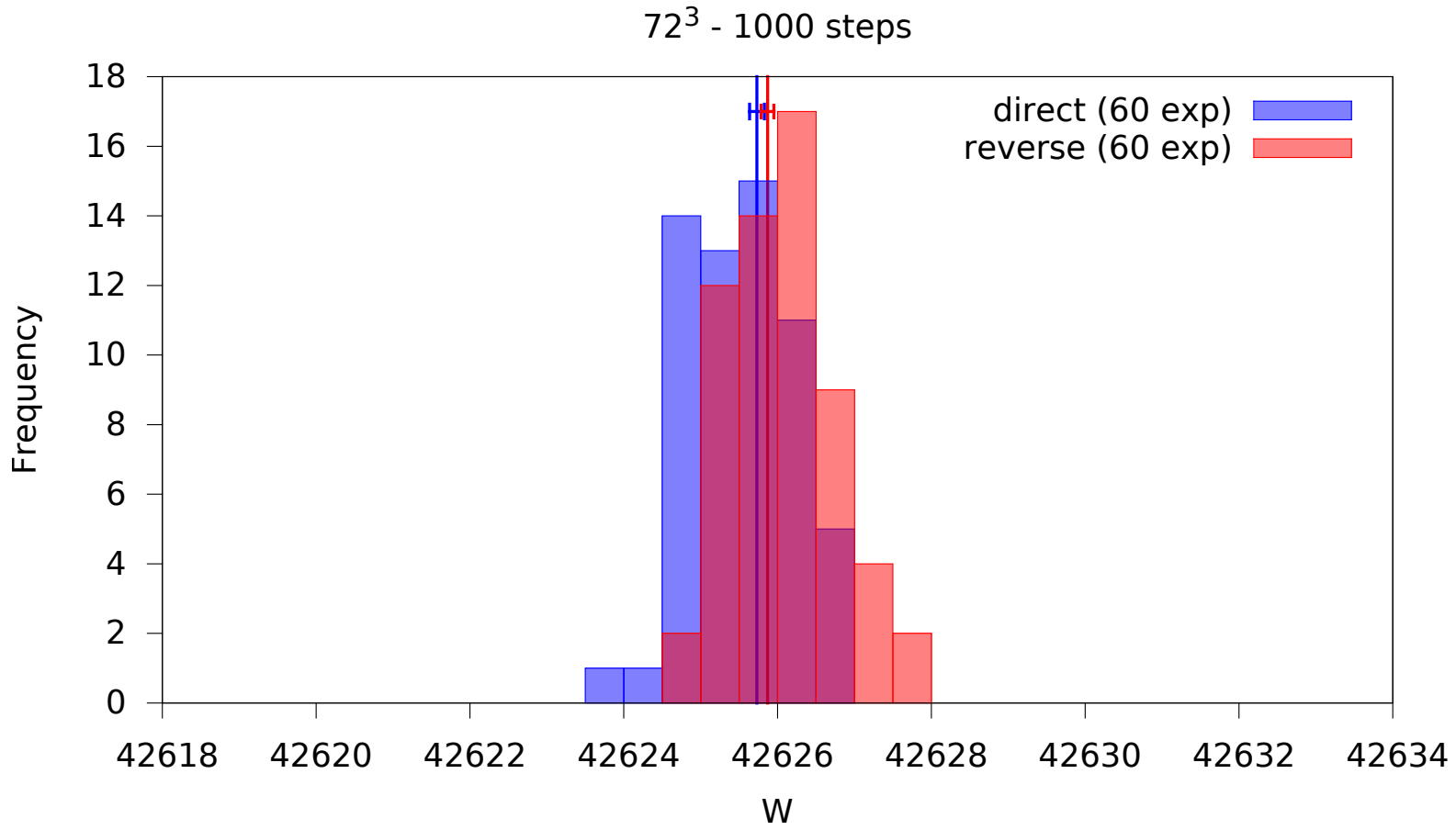
Dominant realizations



Picture taken from [Jarzynski (2006)]

In most realizations the work is statistically distributed on $\rho(W)$; however the trials that dominate the exponential average are in the region where $g(W) = \rho(W)e^{-\beta W}$ has the peak.

Work histograms



Values of total work W for different transformations $\beta = 2.4158 \leftrightarrow 2.4208$ for $N_t = 6$ in $\mathrm{SU}(2)$ theory. Vertical lines indicate the value of the free energy difference ΔF obtained from these trials (with the corresponding error).

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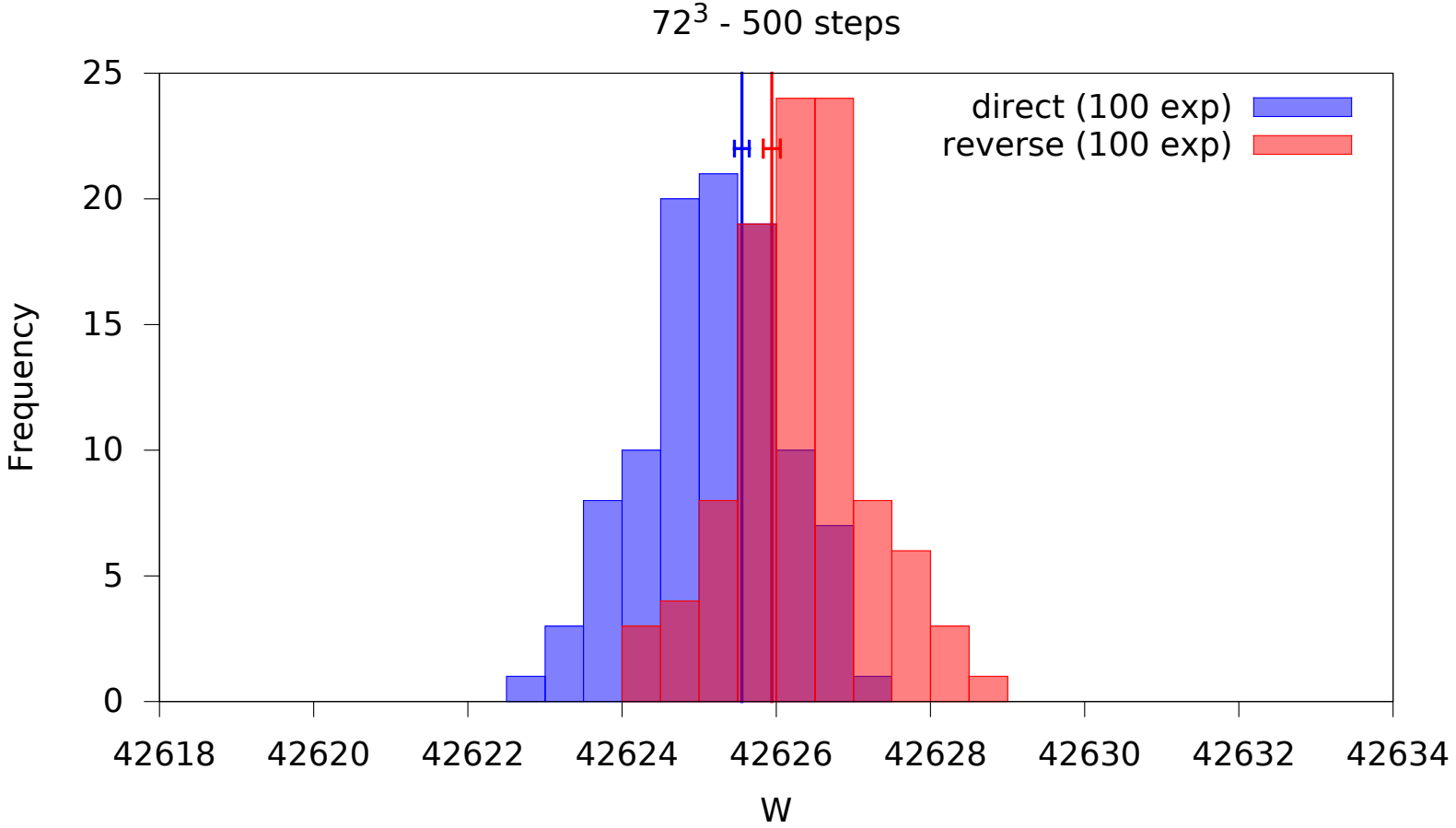

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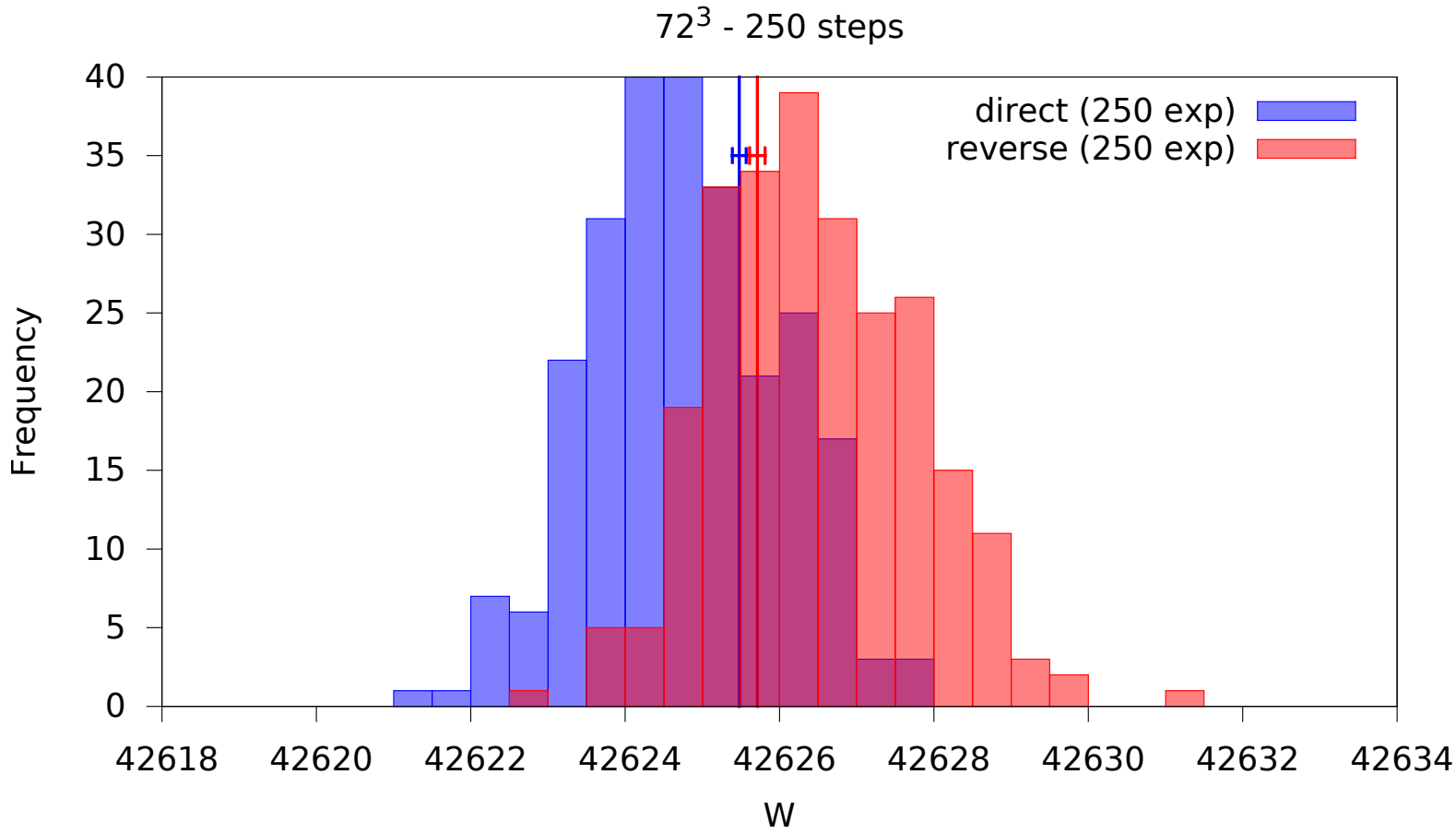

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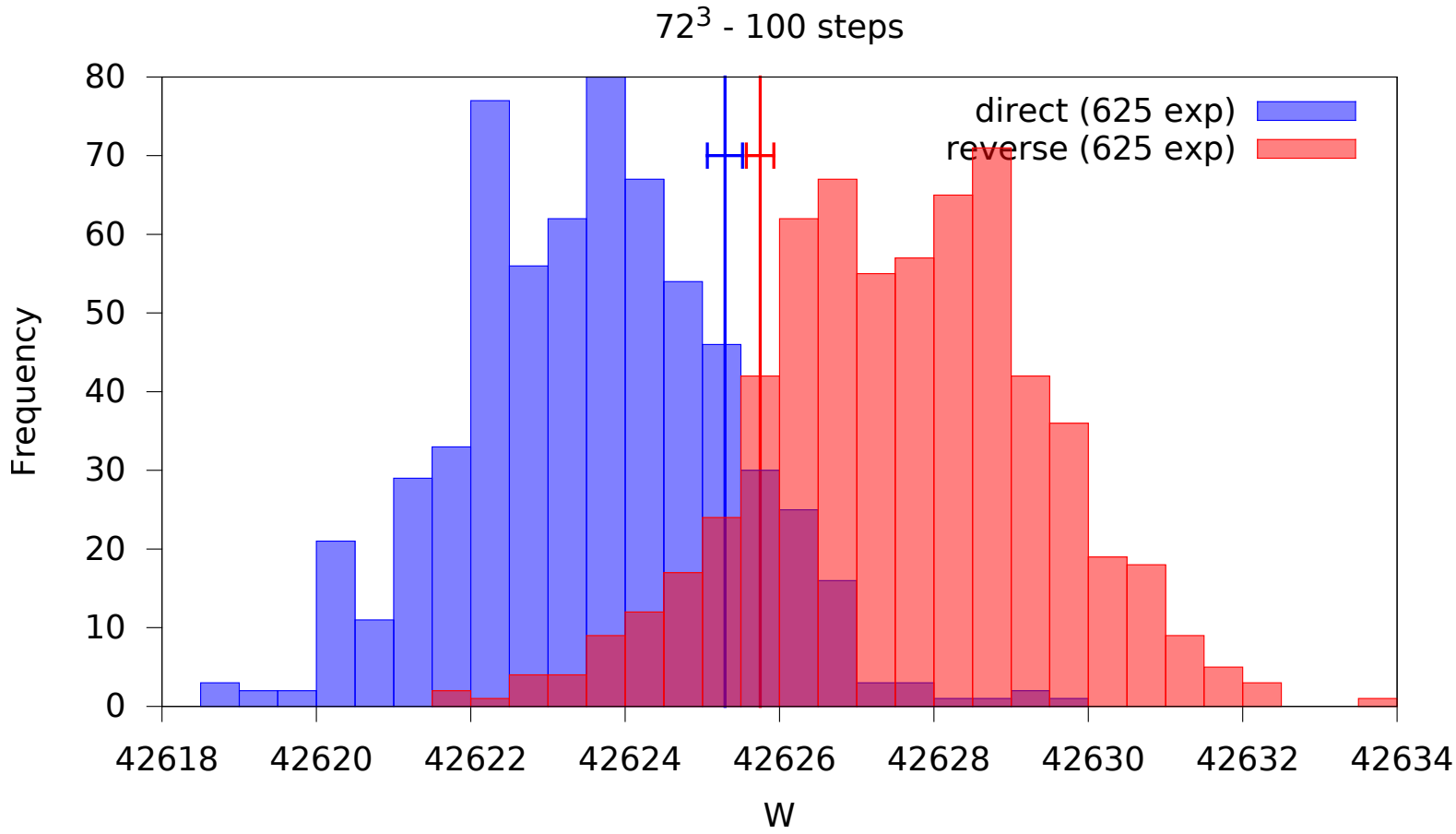

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Eliminating the vacuum contribution

The pressure is normalized to the value of $p(T)$ at $T = 0$ in order to remove the contribution of the vacuum. Using the 'integral method' the pressure can be rewritten (relative to its $T = 0$ vacuum contribution) as

$$\frac{p(T)}{T^4} = -{N_t}^4 \int_0^\beta d\beta' \left[3(P_\sigma + P_\tau) - 6P_0\right]$$

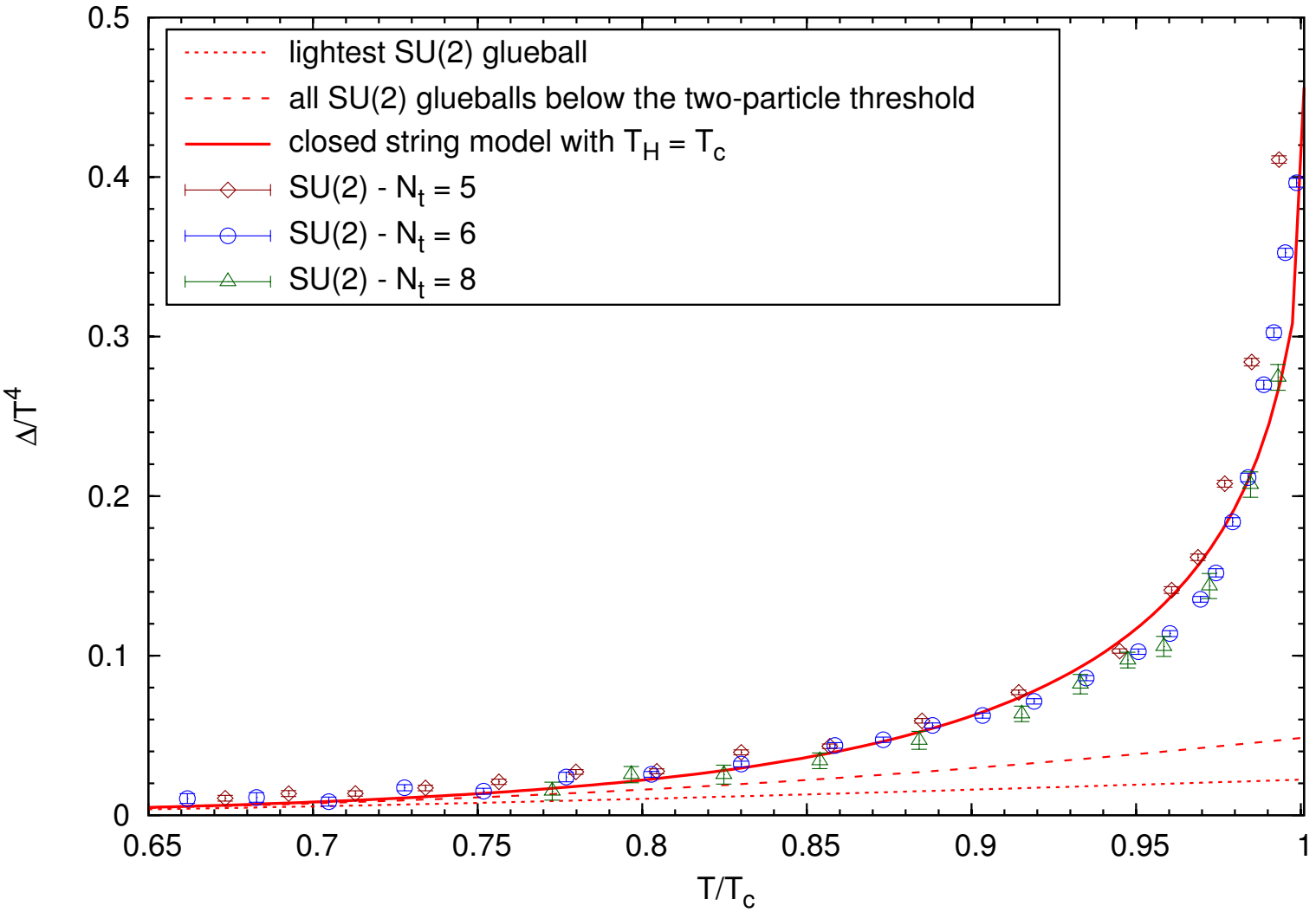
where P_σ and P_τ are the expectation values of spacelike and timelike plaquettes respectively and P_0 is the expectation value at zero T.

Using Jarzynski's relation one has to perform another transformation $\beta_i \to \beta_f$ but on a symmetric lattice, i.e. with lattice size $\widetilde{N}_s^4$ instead of $N_t \times N_s^3$. The finite temperature result is then normalized by removing the $T = 0$ contribution calculated this way.

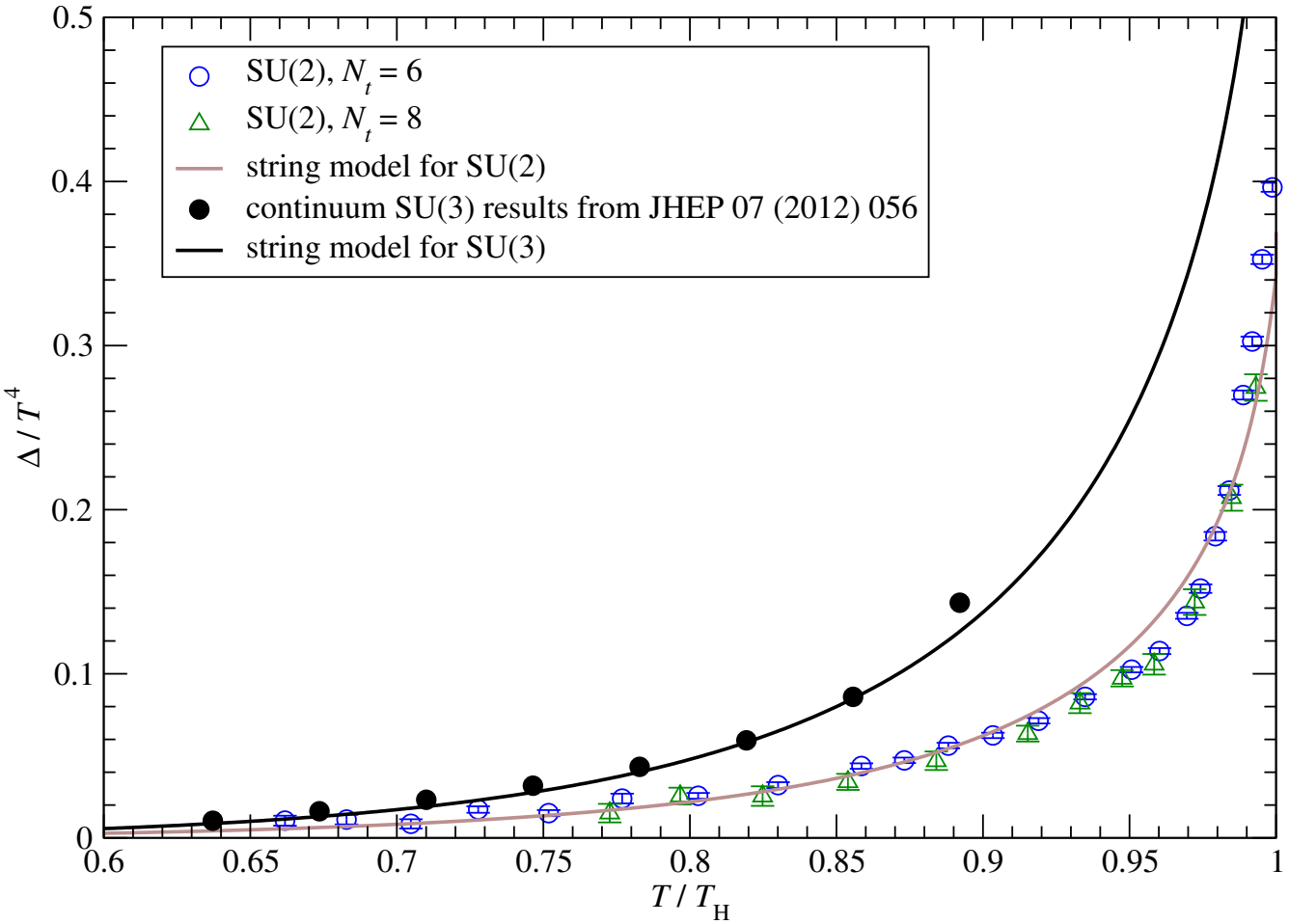
$$\frac{p(T)}{T^4} = \frac{p(T_0)}{T_0^4} + \left(\frac{N_t}{N_s}\right)^3 \ln \frac{\left\langle \exp\left[-W_{\mathrm{SU}(N_c)}(\beta_g^{(0)}, \beta_g)_{N_t \times N_s^3}\right]\right\rangle}{\left\langle \exp\left[-W_{\mathrm{SU}(N_c)}(\beta_g^{(0)}, \beta_g)_{\widetilde{N}^4}\right]\right\rangle^\gamma}$$

with $\gamma = \left(N_s^3 \times N_0\right) / \widetilde{N}^4$.

Hagedorn spectrum in SU(2) pure gauge theory



Hagedorn spectrum in SU(2) and SU(3) pure gauge theories



Jarzynski's relation for non-isothermal transformations

$$\left\langle \exp\left(-\sum_{n=0}^{N-1} \left\{ \frac{H_{\lambda_{n+1}}\left[\phi_n\right]}{T_{n+1}} - \frac{H_{\lambda_n}\left[\phi_n\right]}{T_n} \right\} \right) \right\rangle = \frac{Z(\lambda_N, T_N)}{Z(\lambda_0, T_0)}$$